$Ba_{1-x}K_xBiO_3$ Revisited

M. Rice

(with additional input from M. Beasley)

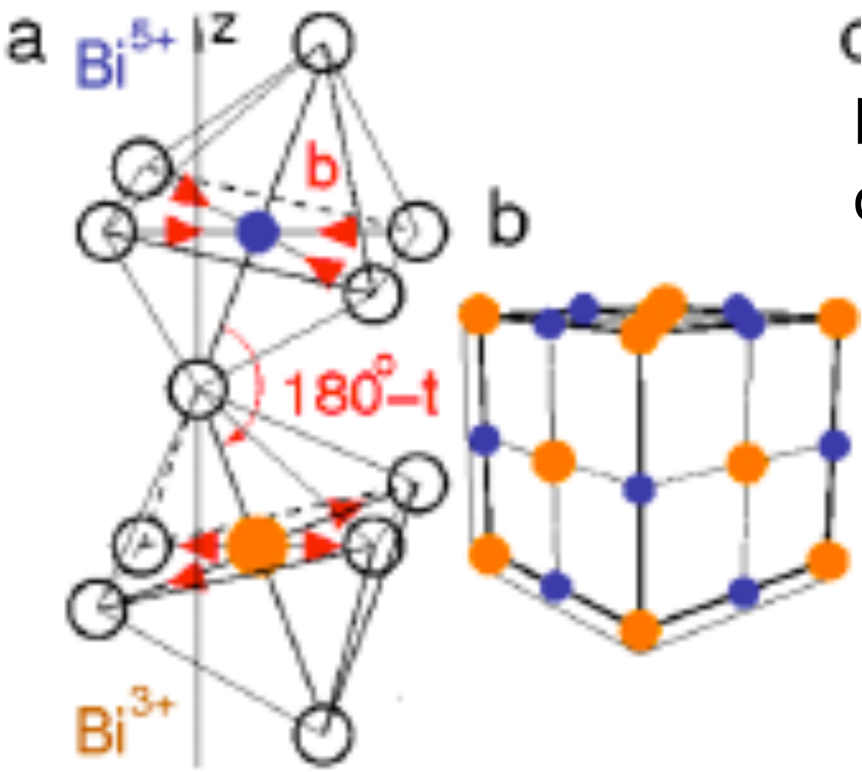
$Ba_{1-x}K_xBiO_3$ Revisited : Discussion Topics

- Origin of CDW order in $BiBaO_3$ with Bi^{3+} & Bi^{5+} local sites
  Coulomb (Varma) or Lattice Forces(Franchini et al PRL`09) ?
  Bi is a Valence Skipper.
- Mechanism of Superconductivity with Tc = 30K in BKBO :
  Negative U or Strong Coupling El-Phonon ?

- Similarites and Contrasts between the two Phase Diagrams
  e.g. SC Tc & Doping Range:
  BKBO (30K & x > 0.4) Cuprates(130K & x> 0.04)

- Anomalous Normal State of BKBO => Low Energy Model ?

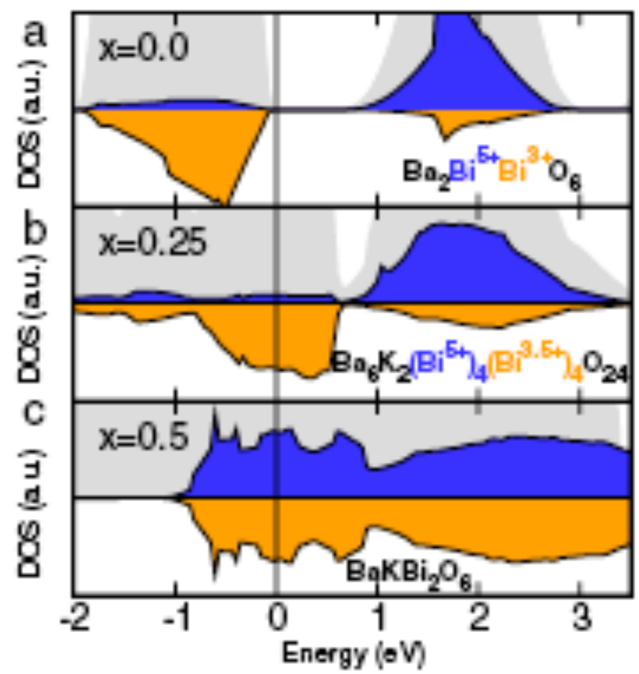
- What can we learn from BKBO about the prospects for a
  Useful High Temperature Superconductor ?



$BaBiO_3$ showing CDW with ordered array of Bi^{3+} & Bi^{5+}

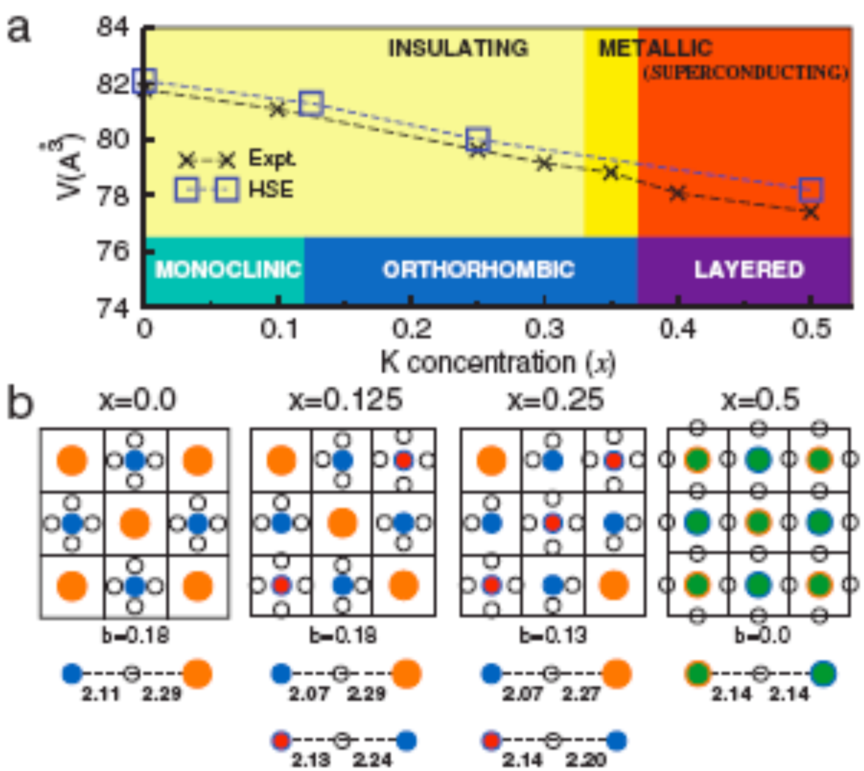
Nonpolaronic DOS for BKBO
Bi^{3+} & Bi^{5+}

Franchini et al PRL `09
using LDA incl SIC

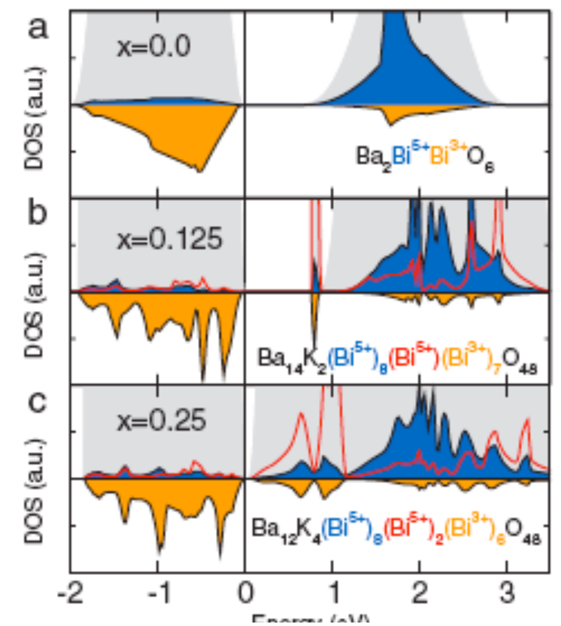


Theory with Superlattice agrees with Expt for Volume , Bi - O distances and ε_2 in BKBO

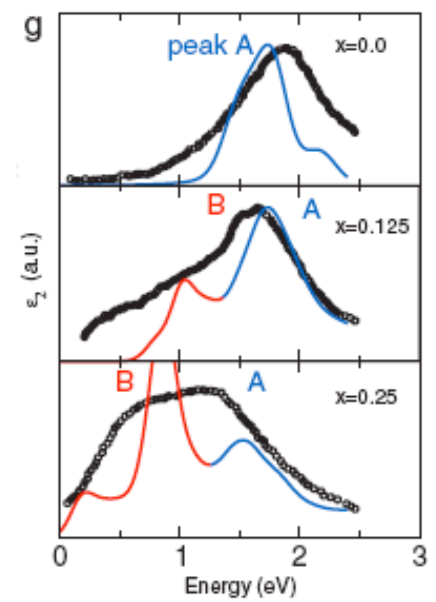
Franchini et al PRL `(



Superlattice DOS



ε_2



Proposed Superlattice Ordering of Bi^{3+} & Bi^{5+} leads to Insulator at x=0.25

=> Bipolaron Formation of Bi^{5+}

Mechanism of the 30K Superconductivity in BKBO

Estimates of El.-Phonon λ too low to give a Tc of 30K

e.g.Meregalli & Savrasov: Standard LDA Estimate λ = 0.34

Marsiglio et al : Eliashberg Analysis of $\sigma(\omega)$ => λ = 0.2

Batlogg et al: Isotope Shift => λ =0.2

So is a value of U < 0 required ?

Or will the SIC LDA revise the estimates ?

Similarities and Contrasts between Bi & Cu Superconductors

BKBO: Max. Tc = 30 K SC when x> xc =0.4

Cuprates: Max Tc = 133K SC when x>xc = 0.04

Is this because Tc (CDW) > T_N and >> Tc(SC) ?

Does it reflect that the coupling to the lattice distortion of local 2el. pairs is classical and but the singlet spin pairs in an AF are quantum fluctuations ?

However both have a low superfluid density & large λ_L

Optical Properties Puchkov et al

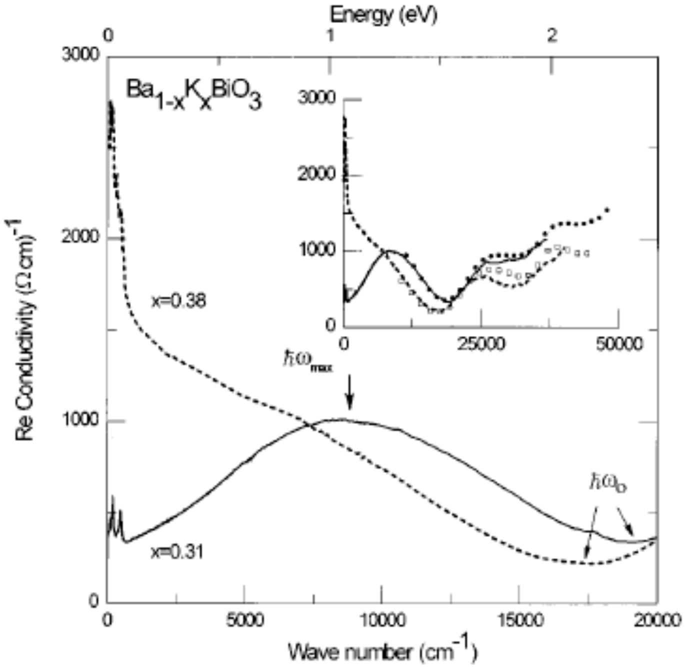


FIG. 1. The optical conductivity of $Ba_{1-x}K_xBiO_3$ just below and just above the insulator-metal transition. The characteristic energies $\hbar\omega_{max}$ and $\hbar\omega_0$, used in the text, are shown. The inset: the lines represent the real part of the optical conductivity obtained from the KK analysis of reflectivity spectra. The symbols show results of ellipsometric measurements.

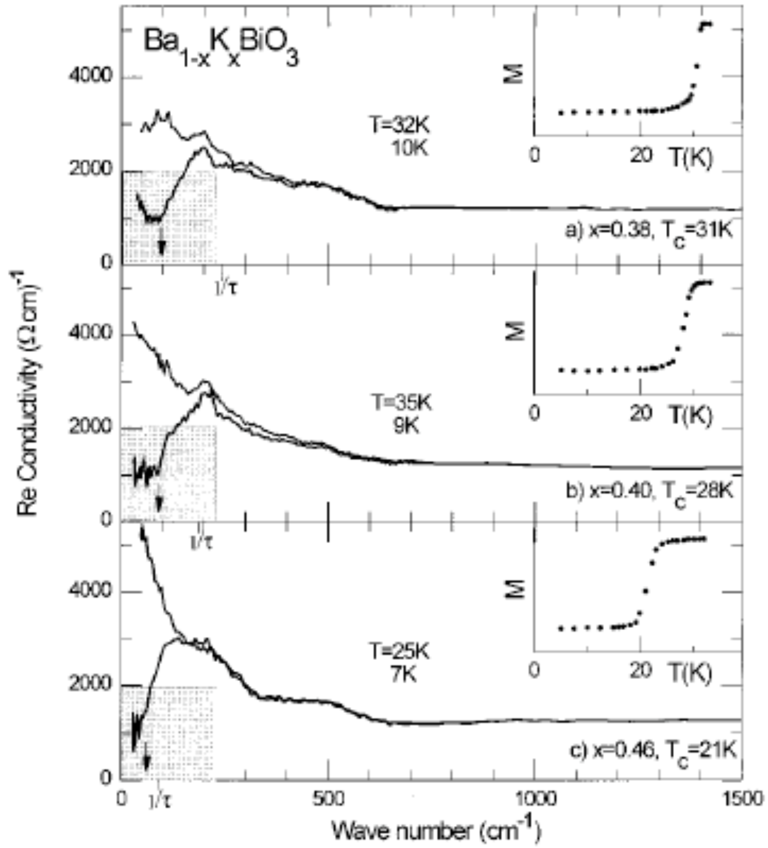


FIG. 4. The optical conductivity of the three metallic samples BKBO in the superconducting and the normal states. The results of magnetization measurements are shown on the insets. The scattering rate values $1/\tau$ in the normal state are shown on the frequency axis for all three samples. The shaded squares represent the spectral weight of the superconducting carriers. The London penetration depth λ_L is inversely proportional to the side of the square. The position of the superconducting gap energy $2\Delta_s$ is shown by the arrows.

Only 3 x 10^{20} carriers in Drude Peak
and little change with x.
Strong MIR peak

Low Energy Model for Normal State ??

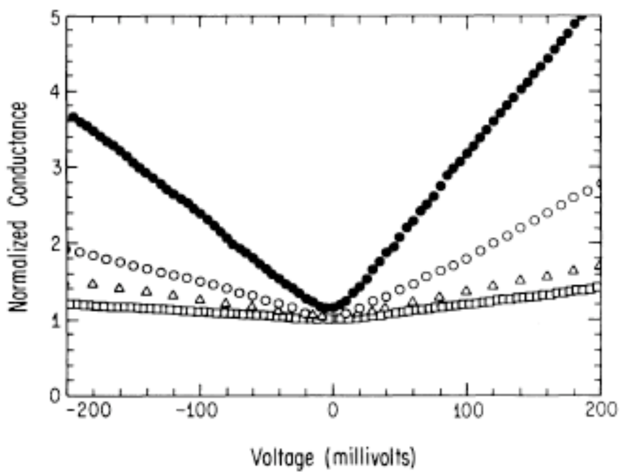


FIG. 3. Normalized conductance for tunnel junctions on BKBO (solid circles), $BaPb_{0.75}Bi_{0.25}O_3$ (open circles), $BaPb_{0.75}Sb_{0.25}O_3$ (triangles), and $BaPbO_3$ (squares) at 1.2 K. Note that the slope of the linear conductance scales with the superconducting transition temperature T_c and that there is an asymmetry of approximately a factor of 2 about zero bias for all four materials.

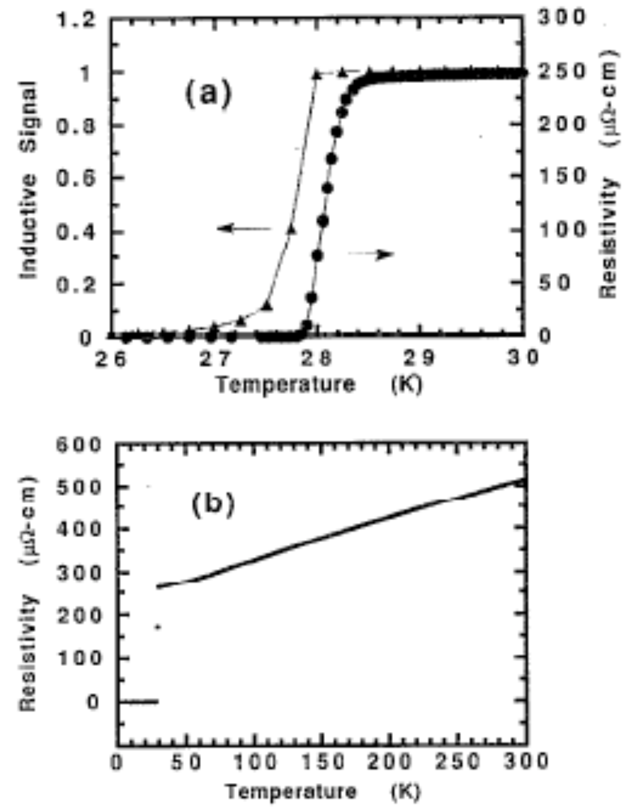
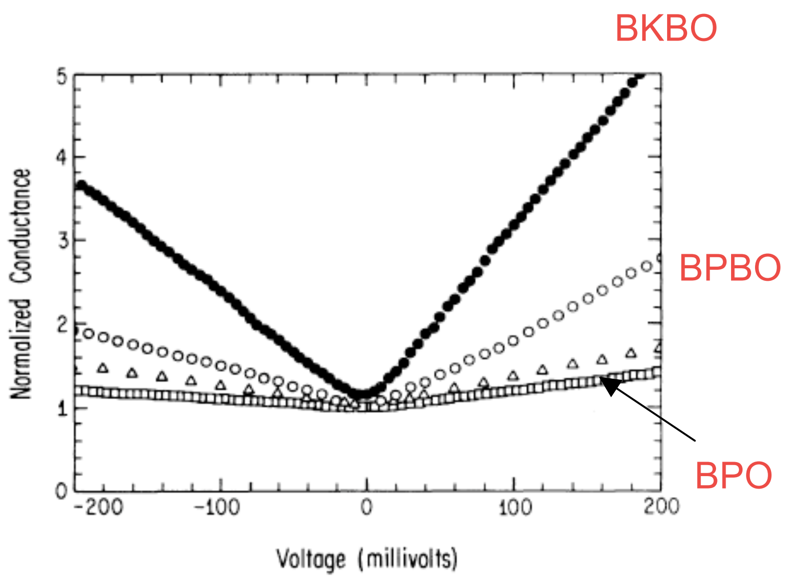


FIG. 1. (a) Comparison of the magnetic screening and resistivity transitions for a DKDO thin film. The onset of the magnetic transition and the zero resistance temperature each occur at 28 K, with transition widths less than 0.5 K. (b) Resistivity vs temperature for a patterned BKBO line. The resistivity is nearly linear from the transition to above room temperature, with residual resistance ratio $\rho(300)/\rho(T_c) \simeq 2$.

Anomalous Tunneling Spectra
Sharifi et al `91

Linear T Resistivity Schweinforth et al `92

CORRELATION BETWEEN SLOPE OF BACKGROUND AND Tc FOR VARIOUS MATERIALS



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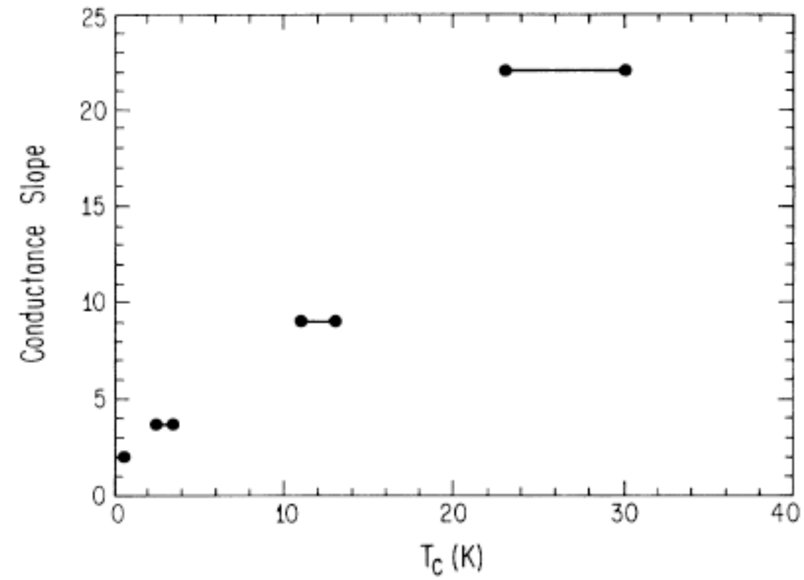

FIG. 4. Magnitude of the slope of the conductance positive bias vs the superconducting transition temperature T_c. Error bars reflect variations of T_c in a particular compound due to stoichiometry differences.

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STRUCTURAL PHASE DIAGRAM

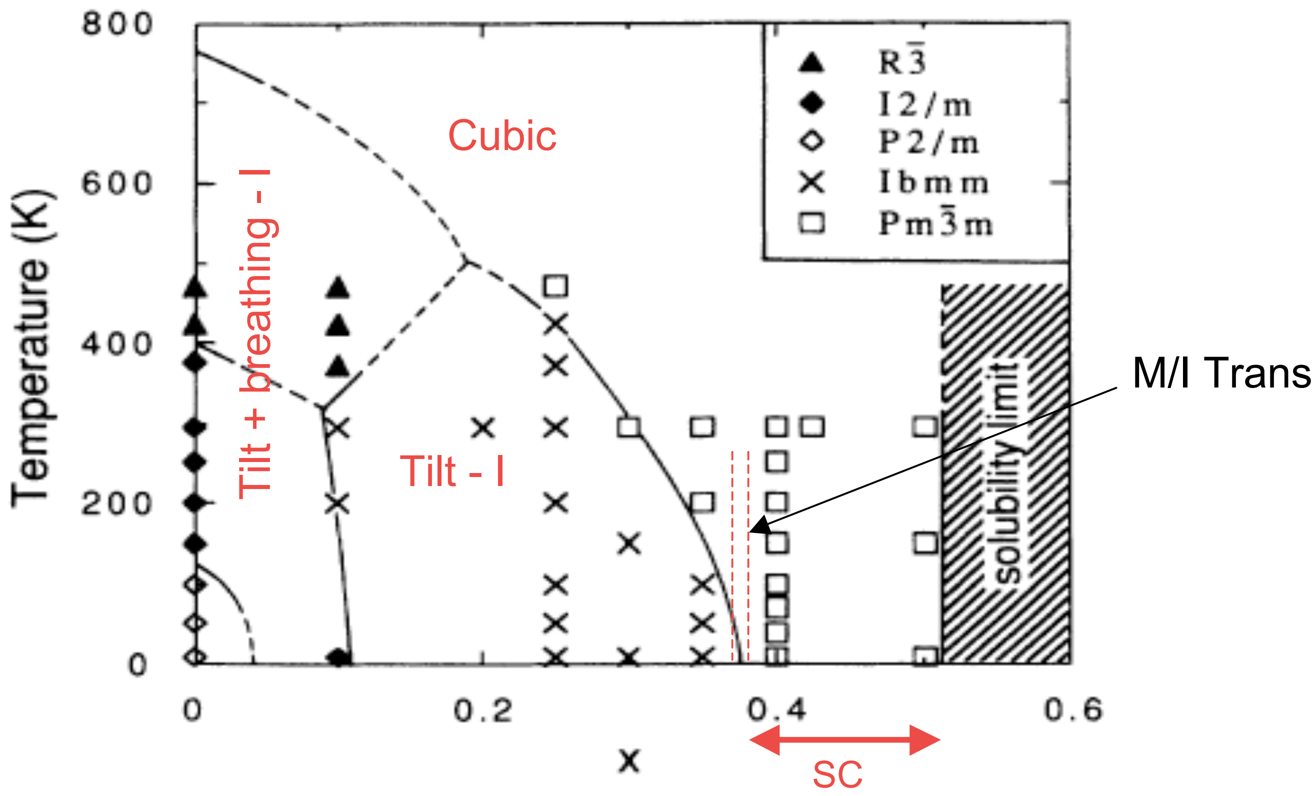


FIG. 3. Phases identified by neutron powder diffraction in the $Ba_{1-x}K_xBiO_3$ ($x \leq 0.5$) system. Each symbol marks a composition and temperature for which a Rietveld structural refinement has been performed. The exact location of the phase boundaries is limited by the number of data.

Tc vs COMPOSITION
(Two studies)

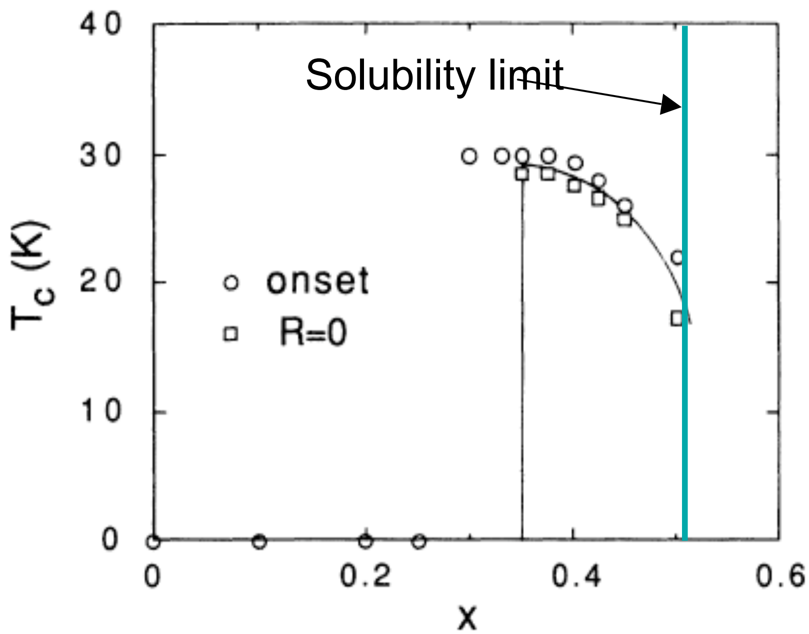


FIG. 2. Superconducting transition temperatures T_c vs x for $Ba_{1-x}K_xBiO_3$. Circles mark the resistive onset temperatures and squares mark the zero-resistance temperatures. Where no square symbols are shown, zero resistance was not reached at any temperature above 10 K.

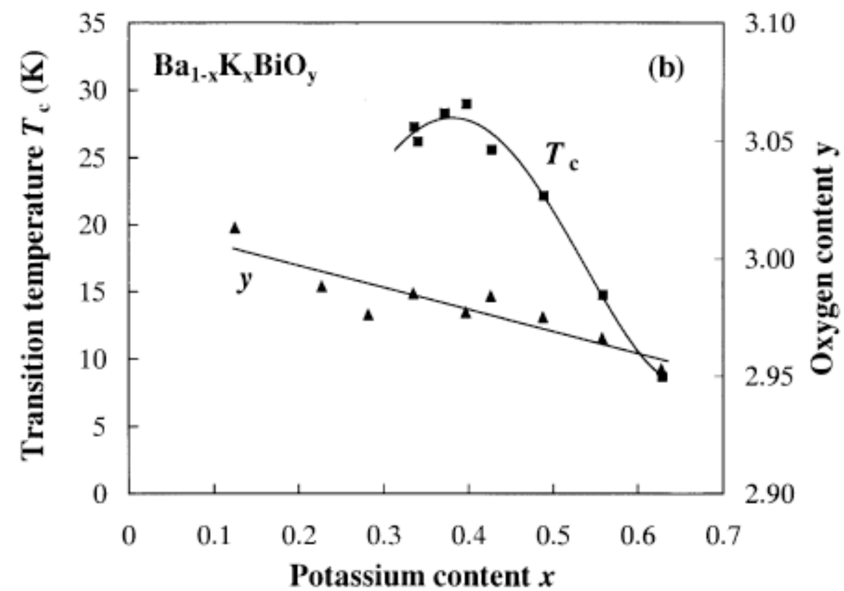
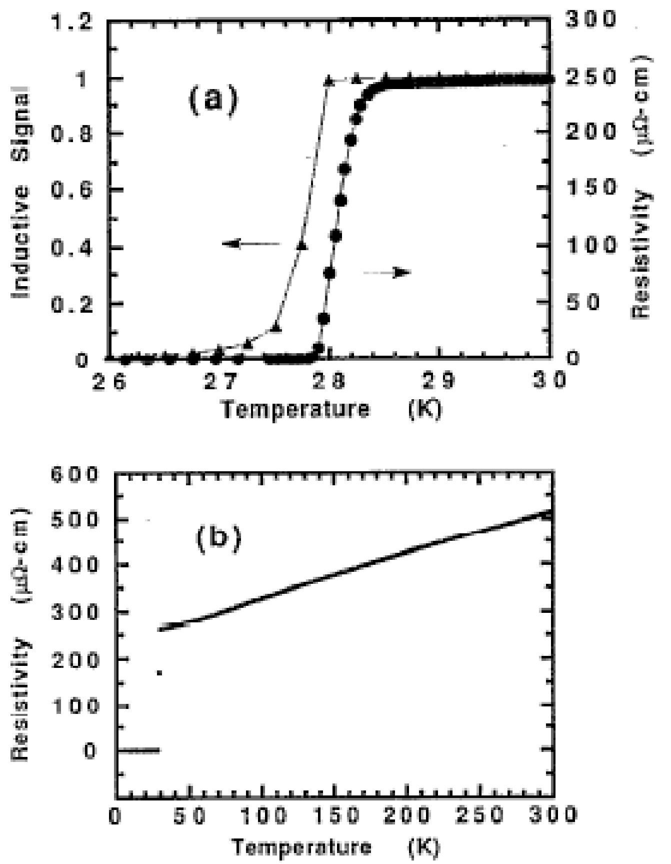


Fig. 1. (a) Potassium content x of $Ba_{1-x}K_xBiO_3$ crystals as a function of weight ratio $Ba(OH)_2 8H_2O/KOH$ in nominal composition. (b) Oxygen content and superconducting critical temperature of the crystals as a function of potassium content. The solid lines are only a visual guide.

Linear Resistivity at Optimal Doping



VanHarlingen

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ANGLE INTEGRATED PHOTO-EMMISSION

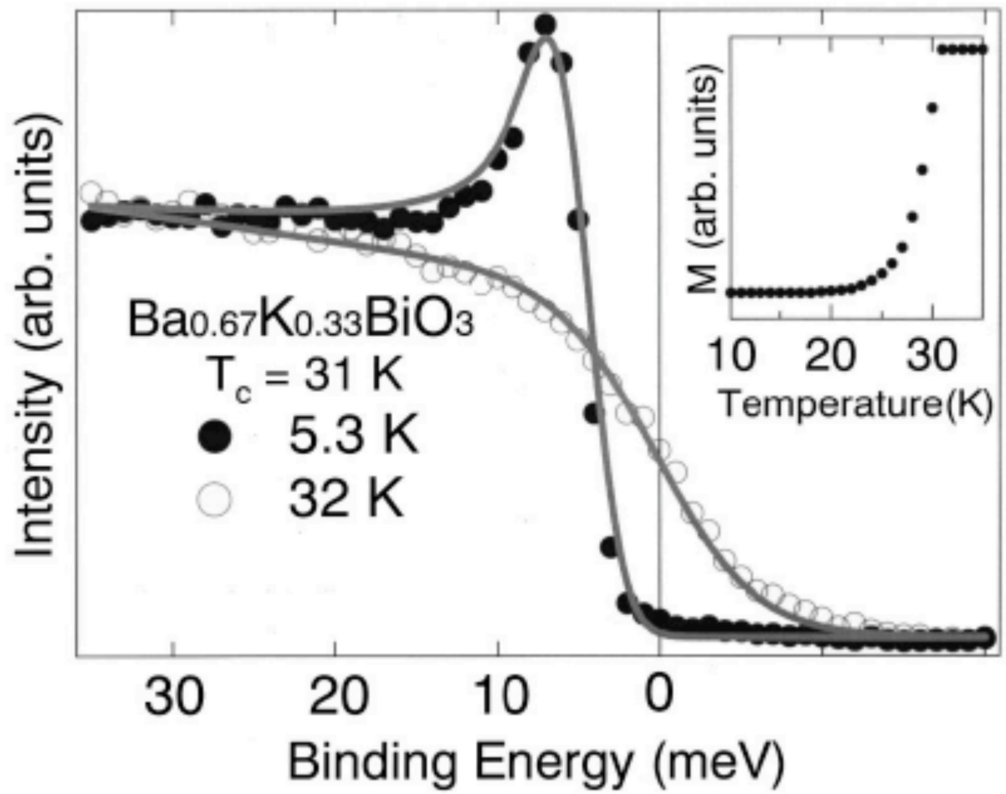


FIG. 1. Ultrahigh resolution photoemission spectra of $Ba_{0.67}K_{0.33}BiO_3$ near E_F (photon source: He Iα, $h\nu = 21.218$ eV) at 5.3 and 32 K. The 5.3 K spectrum shows a clear superconducting gap. The lines are fits to the normal and superconducting states (see text). Inset: magnetization vs T.

TEMPERATURE DEPENDENCE OF GAP

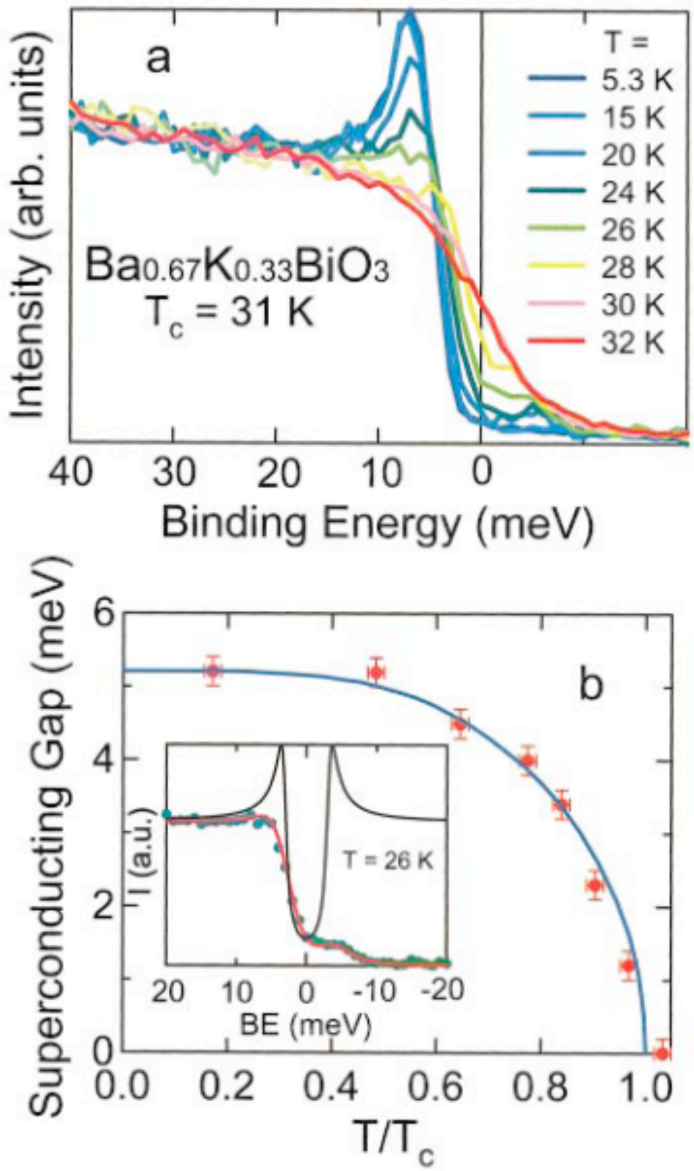
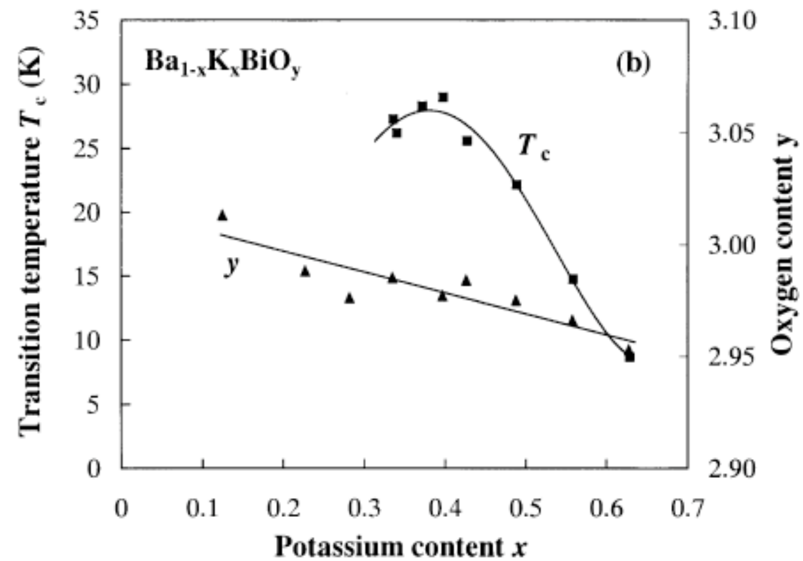


FIG. 2. (Color) (a) The temperature dependent spectra exhibit a systematic pileup in the DOS. (b) Experimental (symbols) and BCS (line) gap vs T/T_c. Inset to (b): the spectrum (symbols) with the fit (red line) for $T = 26$ K. The small peak above E_F originates in the superconducting DOS (black line).



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PSEUDO-GAP

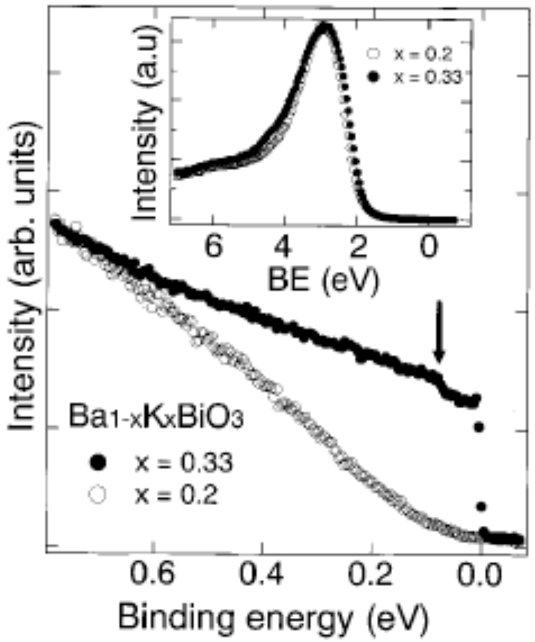
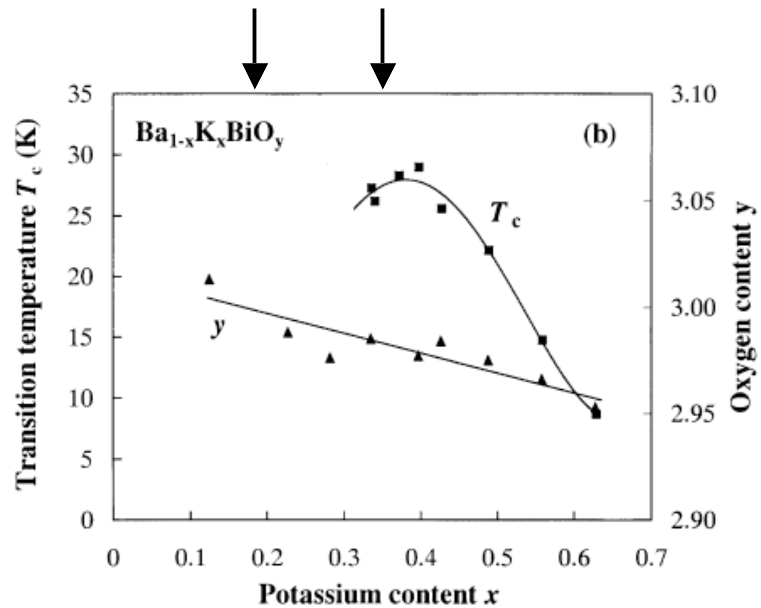


FIG. 3. The valence band spectra of $Ba_{1-x}K_xBiO_3$ ($x=0.2$ and 0.33) showing changes across the semiconductor-metal transition and a pseudogap over ~70 meV (arrow) for $x=0.33$ at 5.3 K. The superconducting transition is not clear here due to the larger step size used. The inset shows the full valence band spectra.



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